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LLNL-TR-738379

Synthesis of a Novel Energetic Heterocyclic Oxidizer with Higher Energy and Lower Sensitivity Final Report CRADA No. TC02099.0

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September 12, 2017

Disclaimer

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Synthesis of a Novel Energetic Heterocyclic Oxidizer with Higher Energy and Lower Sensitivity

Final Report
CRADA No. TC02099.0
Date Technical Work Ended: January 10, 2007

Date: January 11, 2007 Revision: 0

A. Parties

This project was a relationship between Lawrence Livermore National Laboratory (LLNL) and Physical Sciences, Inc. (PSI).

The Regents of the University of California
Lawrence Livermore National Laboratory
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Livermore, CA 94550
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Physical Sciences, Inc.
20 New England Business Center
Andover, MD 01810-1077
Ana Racoveanu
Tel: (978) 738-8232
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B. Project Scope

The project involved the synthesis of 5g of a target energetic compound, 3,4-bis(5-nitro-1,2,5-oxadiazol-4-yl)-1,2,5-oxadiazole-1-oxide (DNTF. The deliverables were the synthesis of 5g of DNTF along with quantities of the precursor compounds. In addition, small-scale safety tests on DNTF were performed, which to confirmed that DNTF has no undesirable safety properties before scaling up the synthesis in Phase II of this project.

This CRADA project was a collaborative effort between The Regents of the University of California, Lawrence Livermore National Laboratory (LLNL) and Physical Sciences, Inc. (PSI), to develop a synthesis of a novel energetic heterocyclic oxidizer with higher energy and lower sensitivity. The project consisted of the following five major tasks and deliverables:

Task 1: Synthesis of 500 mg of 3,4-diaminofurazanfuroxan (DATF) - PSI (Months 1-3)

Task 2: PSI will synthesize 5 g of 3,4-diaminofurazanfuroxan (DATF - PSI (Months 3-4)

Task 3: Oxidation of 3,4-diaminofurazanfuroxan (3) to 3,4-dinitrofurazanfuroxan (DNTF) and shipping sample to Aerojet Corp.- LLNL (Month 5)

Task 4: Testing of DNTF – Small-scale safety tests, thermal stability tests and performance testing will be performed by Aerojet Corp. - LLNL/Aerojet (Months 5-6)

Task 5: Management and Reporting - PSI (Months 7-10)

Deliverables:

1. PSI will synthesize 5-10g of DATF - due Month 4 (PSI)
2. LLNL will synthesize 5g of DNTF - due Month 5 (LLNL)
3. LLNL will ship DNTF to Aerojet for testing - due Month 6 (LLNL)
4. Aerojet will perform small-scale safety and performance tests on 5g of DNTF - due Month 7. (LLNL/Aerojet)
5. Final Technical Report due upon completion of the project. (PSI)
6. Final Report and Abstract due within thirty (30) days of completion or termination of the project, as required under Article XI of the CRADA. (LLNL/PSI)

This CRADA was designated as a ten (10) month project. All tasks and deliverables were successfully completed on time.

C. Technical Accomplishments

The specific accomplishments of this project were the synthesis of 5g of DNTF, completion of the small-scale safety tests and a confirmation that the scale-up of DNTF is warranted.

D. Expected Economic Impact

The development of this new energetic material may lead to the development of new propellant formulations which may be incorporated in new weapon systems. The scale-up and development of the new propellant formulation would employ a significant amount of people and require a significant amount of research and development work. The primary commercial application of the oxidizer developed under this CRADA is as an ingredient in a tactical weapon system.

D.1 Specific Benefits

Benefits to DOE

This CRADA benefits DOE by increasing LLNL's expertise in energetic materials. Such knowledge is frequently important for our core mission. In addition, this technology could help the DOD by creating a new propellant material. In addition, if the technology works for DOD applications, it could eventually find its way to the commercial sector for selected applications.

Benefits to Industry

The U.S. taxpayer will benefit from both the DOD and potential commercial applications.

E. Partner Contribution

PSI supplied the precursor compound, 3,4-bis(5-amino-1,2,5-oxadiazol-4-yl)-1,2,5-oxadiazole-1-oxide (DATF). Aerojet performed the performance measurements and predictions. PSI also completed the final report for our sponsors.

F. Documents/Reference List

Reports

PSI completed a report to the sponsor describing the accomplishments under the contract.

Copyright Activity

None

Subject Inventions

None

Background Intellectual Property

No Background Intellectual Property was disclosed by either party.

G. Acknowledgement

Industrial Participant's signature of the final report indicates the following:

1) The Participant has reviewed the final report and concurs with the statements made therein.
2) The Participant agrees that any modifications or changes from the initial proposal were discussed and agreed to during the term of the project.
3) The Participant certifies that all reports either completed or in process are listed and all subject inventions and the associated intellectual property protection measures generated by his/her respective company and attributable to the project have been disclosed and included in Section E or are included on a list attached to this report.
4) The Participant certifies that if tangible personal property was exchanged during the agreement, all has either been returned to the initial custodian or transferred permanently.
5) The Participant certifies that proprietary information has been returned or destroyed by LLNL.

A Racoveanu — April 11, 2007

Ana Racoveanu — Date
Physical Sciences, Inc.

Philip Pagoria — May 1, 2007

Phillip Pagoria, LLNL Principal Investigator — Date
Lawrence Livermore National Laboratory

Karena McKinley — 5/10/07

Karena D. McKinley, IPAC Director — Date
Lawrence Livermore National Laboratory

Attachment I – Final Abstract

Synthesis of a Novel Energetic Heterocyclic Oxidizer with Higher Energy and Lower Sensitivity

Final Abstract (Attachment I)
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B. Purpose and Description

The project involved the synthesis of 5g of a target energetic compound, 3,4-bis(5-nitro-1,2,5-oxadiazol-4-yl)-1,2,5-oxadiazole-1-oxide (DNTF. The deliverables were the synthesis of 5g of DNTF along with quantities of the precursor compounds. In addition, small-scale safety tests on DNTF were performed, which confirmed that DNTF has no undesirable safety properties. These results led to the awarding of a Phase II of this project that will involve a scale-up of DNTF to the 100g scale.

All tasks and deliverables were successfully completed on time.

C. Benefit to Industry

The U.S. taxpayer will benefit from both the DOD and potential commercial applications.

D. Benefit to DOE/LLNL

This CRADA benefits DOE and LLNL by expanding our expertise in energetic materials. Such knowledge is frequently important for our core mission. In addition, this technology could help the DOD by creating a new propellant material. In addition, if the technology works for DOD applications, it could eventually find its way to the commercial sector for selected applications.

E. Project Dates

March 10, 2006 to January 10, 2007.